# Metric deformation and eigenvalue problem in 2D for an irregular boundary

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We prescribe a new formulation for solving the Helmholtz equation in 2D with irregular boundary. A suitable diffeomorphism is used to annul the asymmetries in the boundary by mapping it into an equivalent circle. This results in a modification of the metric in the interior of the region and manifests itself in the appearance of new gauge dependent source terms in the original homogeneous equation. The modified equation is then solved perturbatively. This method allows us to retain the simple form of the boundary condition at the cost of complicating the form of the original equation. It is seen to work reasonably well even for boundaries with large deviations from a circle by comparing our results with the exactly/numerically obtained ones. The Fourier representation of the boundary ensures the convergence of the perturbation series.

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*Introduction.*— The two dimensional Helmholtz equation appears in a wide range of physical and engineering problems across diverse fields − like the study of vibration, acoustic and electromagnetic wave propagation and quantum mechanics. In a large class of these problems one is required to determine the eigenspectrum of the Helmholtz operator for various boundary conditions and geometries. Analytic closed-form solution to the eigenvalue problem [1] can however be obtained only for a restricted class of boundaries. Invoking the geometry of the problem by a suitable choice of co-ordinates often aids in finding the solutions (e.g. elliptic boundary where, separation of variables lead to a solution in the form of Mathieu functions). However, one quickly exhausts the list of such problems where simplification by virtue of using a specific co-ordinate system is possible. In most physical problems, one encounters boundaries which are far removed from such idealization like the case of the quantum dot. The dots are believed to be circular but in practice that can hardly be guaranteed. In such a scenario it is natural to consider the confining region to be a supercircle [2]. Further, the problem gets analytically intractable for irregular boundaries.

The problem of solving Helmholtz equation for an irregular boundary has mostly been tackled using numerical methods [3]. The analytic approach towards this has mainly revolved around various approximation methods. Of these, the perturbative techniques stand out as being the most widely used [1, 4]. The work by [5] study irregular domains in a general formalism using Fourier representation of the boundary asymmetry treated as a perturbation around an equivalent circle.

We have explored an alternative approach towards solving the eigenvalue problem for the two dimensional Helmholtz operator in the interior of a region bounded by an irregular closed curve. The general problem is mapped into an equivalent problem where the boundary is a regular closed curve (for which the Helmholtz equation is exactly solvable) whereas the equation itself gets modified owing to the deformation of the metric in the interior. The modified equation, we see, can be written as the original Helmholtz equation with additional terms arising from perturbation in the metric. The extra pieces can now be treated as a perturbation to the original Helmholtz operator. The equation is thereby solved using the Schrödinger perturbation technique [6]. The corrections to the eigenvalues and the eigenfunctions are expressed in a closed form at each order of perturbation. In this approach towards solving the equation, the boundary conditions are specified on some known regular curve and maintain the same simple form throughout. This bypasses the issue of imposing constraints on a boundary having a complicated geometry.

We expect this perturbative scheme to effectively solve the eigenvalue problem for boundaries which reflect slight departure from known regular curves. We have verified our method against the numerically obtained solutions for a square (exact), an ellipse and a supercircle [7]. In this analysis we use Fourier representation of the perturbations. This allows us to apply the method to a general class of continuous or discontinuous asymmetries.

*Formulation.*— The homogeneous Helmholtz equation on a 2 dimensional flat simply connected surface $\mathcal{S}$ reads,

$$\left(g^{ij}\nabla_i\nabla_j + k^2\right)\psi = 0, \tag{1}$$

where $\nabla$ represents a covariant derivative. We look for solutions in the interior of the bounded region with the Dirichlet condition $\psi = 0$ on the boundary $\partial\mathcal{S}$. The parameter $k^2$ may be identified as $k^2 = E$ for the quantum mechanical problem of a particle confined in the region having energy $E$.

It is convenient to work in polar coordinate system $(r, \theta)$, where any closed curve satisfies the periodicity

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condition $r(\theta) = r(\theta + 2\pi)$. We consider a general irregular boundary of the form $r = r(\theta)$. In this analysis we assume that the arbitrary boundary can be expressed as a perturbation around an effective circle (the analysis can in principle work for a deformation around any simple curve for which the Helmholtz equation is exactly solvable). We introduce new coordinates $(R, \alpha)$ with the transformation $(r, \theta) \to (R, \alpha)$ given by

$$r = R + \epsilon f(R, \alpha) \quad \& \quad \theta = \alpha, \tag{2}$$

where $\epsilon$ is a deformation parameter. This defines a diffeomorphism for the entire class of well behaved functions $f(R, \alpha)$. A suitable choice of $f(R, \alpha)$, shall transform our irregular boundary into a circle of fixed radius, say $R = R_0 (= \frac{1}{2\pi}\int_0^{2\pi} r(\theta)\, d\theta)$ in the $R - \alpha$ plane. The deformation of the irregular boundary to a circle changes the components of the underlying metric $g_{ij}(r, \theta)$ in the interior ($g_{ij}(r, \theta) \to \tilde{g}_{ij}(R, \alpha)$).

The flat background metric in the $(r, \theta)$ system is given by $g_{ij} = \mathrm{diag}(1, r^2)$. Under the coordinate transformations (2) this takes the form

$$\tilde{g}_{ij} = \begin{bmatrix} \left(1 + \epsilon f^{(1,0)}\right)^2 & \epsilon f^{(0,1)}\left(1 + \epsilon f^{(1,0)}\right) \\ \epsilon f^{(0,1)}\left(1 + \epsilon f^{(1,0)}\right) & (R + \epsilon f)^2 + \epsilon^2 {f^{(0,1)}}^2 \end{bmatrix},$$

where $f^{(1,0)} = \frac{\partial f}{\partial R}$ and $f^{(0,1)} = \frac{\partial f}{\partial \alpha}$. Here $f$ and all its derivatives are expressed as functions of $(R, \alpha)$ (dependence on the arguments are not shown explicitly for brevity). We note that except for $\Gamma^{\alpha}{}_{RR} = 0$, all the components of connection $\Gamma$ are non-vanishing. The diffeomorphism (2) does not induce any spurious curvature in the manifold (Riemann tensor, $R^{i}{}_{jkl} = 0$).

The Eq. (1), where $\psi = \psi(r, \theta)$, transforms under the map $(r, \theta) \to (R, \alpha)$ to

$$\begin{aligned} &\frac{\psi^{(0,2)}}{(R+\epsilon f)^2} - \frac{2 f^{(0,1)} \psi^{(1,1)} \epsilon}{(R+\epsilon f)^2 \left(\epsilon f^{(1,0)} + 1\right)} \\ &+ \frac{2 f^{(0,1)} \psi^{(1,0)} \left[(R+\epsilon f) f^{(1,1)} - f^{(0,1)}\left(\epsilon f^{(1,0)} + 1\right)\right] \epsilon^2}{(R+\epsilon f)^3 \left(\epsilon f^{(1,0)} + 1\right)^2} \\ &- \frac{\left[(R+\epsilon f)^2 + \epsilon^2 {f^{(0,1)}}^2\right] \psi^{(1,0)} f^{(2,0)} \epsilon}{(R+\epsilon f)^2 \left(\epsilon f^{(1,0)} + 1\right)^3} \\ &+ \frac{\left[(R+\epsilon f)^2 - \epsilon f^{(0,2)} (R+\epsilon f) + 2\epsilon^2 {f^{(0,1)}}^2\right] \psi^{(1,0)}}{(R+\epsilon f)^3 \left(\epsilon f^{(1,0)} + 1\right)} \\ &+ \frac{\left[(R+\epsilon f)^2 + \epsilon^2 {f^{(0,1)}}^2\right] \psi^{(2,0)}}{(R+\epsilon f)^2 \left(\epsilon f^{(1,0)} + 1\right)^2} + E\psi = 0\,, \end{aligned} \tag{3}$$

where $\psi^{(2,0)} = \frac{\partial^2 \psi}{\partial R^2}$, $\psi^{(0,2)} = \frac{\partial^2 \psi}{\partial \alpha^2}$ and $\psi^{(1,1)} = \frac{\partial^2 \psi}{\partial R \partial \alpha}$. Here $\psi$ and all its derivatives are also expressed as functions of $(R, \alpha)$.

The analysis can proceed from here for a specific form of the function $f(R, \alpha)$. We choose $f(R, \alpha) = Rg(\alpha)$, where $g(\alpha)$ can be expanded without a loss of generality in a Fourier series. We further impose $g(\alpha) = g(-\alpha)$ for simplicity whereby only the cosine terms are retained

$$g(\alpha) = \sum_{n=1}^{\infty} C_n \cos n\alpha. \tag{4}$$

The constant part $C_0$ can always be absorbed in $R$ (2). With this choice of $f(R, \alpha)$, Eq. (3) simplifies to

$$\sum_{n=0}^{\infty} \epsilon^n \mathcal{L}_n \psi + E\psi = 0, \tag{5}$$

where the operator $\mathcal{L}_n$ is given by

$$\begin{aligned} \mathcal{L}_n\psi =& (-1)^n \frac{(n+1)}{6R^2} g^{n-2} \Big[ 3nRg \left\{ g'' \psi^{(1,0)} + 2g' \psi^{(1,1)} \right\} \\ &+ n(n-1) R {g'}^2 \left\{ 2\psi^{(1,0)} + R\psi^{(2,0)} \right\} \\ &+ 6g^2 \left\{ \psi^{(0,2)} + R\psi^{(1,0)} + R^2 \psi^{(2,0)} \right\} \Big]. \end{aligned} \tag{6}$$

In the above equation a prime denotes a derivative with respect to $\alpha$.

We shall adopt the method of stationary perturbation theory [6] to solve for $\psi$ and $E$. Thereby, treating $\epsilon$ as a perturbation parameter we expand the eigenfunction $\psi$ corresponding to the eigenvalue $E$ as

$$\begin{aligned} \psi &= \psi^{(0)} + \epsilon\psi^{(1)} + \epsilon^2 \psi^{(2)} + \cdots; \\ E &= E^{(0)} + \epsilon E^{(1)} + \epsilon^2 E^{(2)} + \cdots, \end{aligned} \tag{7}$$

with superscripts denoting the order of perturbation. We assume that the perturbative scheme converges and $(\psi, E)$ can be calculated order by order up to any arbitrarily desired precision. We note that the parameter $\epsilon$ is arbitrarily invoked to track different orders and could be absorbed in the Fourier coefficients $C_n$.

Plugging (7) in (5), and collecting the coefficients for different powers of $\epsilon$ yields

$$\mathcal{O}(\epsilon^0): \quad (\mathcal{L}_0 + E^{(0)})\psi^{(0)} = 0 \tag{8a}$$

$$\mathcal{O}(\epsilon^1): \quad (\mathcal{L}_0 + E^{(0)})\psi^{(1)} + (\mathcal{L}_1 + E^{(1)})\psi^{(0)} = 0 \tag{8b}$$

$$\cdots$$

$$\mathcal{O}(\epsilon^m): \quad \sum_{n=0}^{m} \left(\mathcal{L}_n + E^{(n)}\right) \psi^{(m-n)} = 0. \tag{8c}$$

The change in the metric components induced by the smooth deformation (2) amounts to a gauge transformation and generates source terms to the unperturbed homogeneous Helmholtz equation at each order in $\epsilon$. At the $i^{th}$ order we have the terms $\mathcal{L}_1\psi^{(0)}, \mathcal{L}_1\psi^{(1)} \cdots, \mathcal{L}_i\psi^{(j(<i))}$, which have no physical origin and are merely artifacts of the chosen gauge. Maintaining the simplicity of Dirichlet boundary condition is hence achieved at the cost of new terms appearing in the original equation.

The unperturbed energy $E^{(0)}$ and corrections $E^{(1)}$, $E^{(2)}$ are given by

$$E^{(0)} = -\langle\psi^{(0)}|\mathcal{L}_0|\psi^{(0)}\rangle; \quad E^{(1)} = -\langle\psi^{(0)}|\mathcal{L}_1|\psi^{(0)}\rangle;$$
$$E^{(2)} = -\langle\psi^{(0)}|\mathcal{L}_1 + E^{(1)}|\psi^{(1)}\rangle - \langle\psi^{(0)}|\mathcal{L}_2|\psi^{(0)}\rangle. \quad (9)$$

A unique feature of our method is that the Dirichlet boundary condition, $\psi^{(i)}(R_0,\alpha) = 0$ maintains its simple form separately for every order in perturbation.

The general solution of the Eq. (8a) is

$$\psi^{(0)}_{l,j} = N_{0,j}J_0(\rho)\,; \qquad (l=0)$$
$$= N_{l,j}J_l(\rho)\left\{\begin{array}{c}\cos(l\alpha)\\ \sin(l\alpha)\end{array}\right\}, \qquad (l\neq 0) \quad (10)$$

where $J_l$ is the $l^{th}$ order Bessel function with the argument $\rho = \sqrt{E^{(0)}_{l,j}}R$ and $N_{l,j}$ is a suitable normalisation constant with $l \in \mathbb{N}$, $j \in \mathbb{N}_{>0}$. The energy spectrum $E^{(0)}_{l,j}$ of the unperturbed Helmholtz equation is dictated by the the $j^{th}$ zero of $J_l$ denoted by $\rho_{l,j}$. Using $\psi^{(0)}_{l,j}(R_0,\alpha) = 0$, we have $E^{(0)}_{l,j} = \rho^2_{l,j}/R^2_0$. In the order of ascending magnitude the energy levels are $E^{(0)}_{0,1}$, $E^{(0)}_{1,1}$, $E^{(0)}_{2,1}$, $E^{(0)}_{0,2}$, $E^{(0)}_{3,1}$, $E^{(0)}_{1,2}$, $E^{(0)}_{4,1}\cdots$, where all the levels with non-zero $l$ are doubly degenerate.

In this formulation the energy corrections can be obtained in two ways. Firstly, $E^{(i)}_{l,j}$ can be estimated from the knowledge of $\psi^{(m)}_{l,j}(\forall\ m<i)$ using Eqs. (9). Alternatively it can be extracted by imposing the boundary condition, $\psi^{(i)}_{l,j}(R_0,\alpha) = 0$ which in addition yields the coefficients of Bessel function (in $\psi^{(i)}_{l,j}$). The method can in principle be used to calculate corrections at all orders of perturbation. We calculate the energy corrections for the following two cases.

*Case I: Non-degenerate states* ($l = 0$)
The first order correction to the eigenfunction is obtained from the Eq. (8b). Thus, we have

$$\psi^{(1)}_{0,j} = a_0J_0(\rho) - \frac{\rho E^{(1)}_{0,j}}{2E^{(0)}_{0,j}}N_{0,j}J_1(\rho) + \sum_{p=1}^{\infty}\Big\{a_pJ_p(\rho) - \rho N_{0,j}C_pJ_1(\rho)\Big\}\cos(p\alpha) \quad (11)$$

The first order energy corrections are obtained by imposing the boundary condition $\psi^{(1)}_{0,j}(R_0,\alpha) = 0$. This yields $E^{(1)}_{0,j} = 0$ and $a_p = \rho_{_{0,j}}N_{0,j}C_pJ_1(\rho_{_{0,j}})/J_p(\rho_{_{0,j}})\,,\ (p\neq 0)$. The vanishing of the first order correction is verified using Eq. (9). The remaining constant $a_0$ can be determined by normalising the corrected wavefunction.

The first non-vanishing energy correction occurs at the second order. The correction $E^{(2)}_{0,j}$ is obtained by substituting $\psi^{(0)}_{0,j}$ and $\psi^{(1)}_{0,j}$ in Eq. (9). We have

$$E^{(2)}_{0,j} = E^{(0)}_{0,j}\sum_{n=1}^{\infty}\xi_{n,j}C_n^2\,; \quad \xi_{n,j} = \frac{1}{2} + \frac{\rho_{_{0,j}}J_n'(\rho_{_{0,j}})}{J_n(\rho_{_{0,j}})}. \quad (12)$$

We may as well solve (8c) for $m = 2$ to obtain

$$\psi^{(2)}_{0,j} = b_0J_0(\rho) - \frac{\rho E^{(2)}_{0,j}}{2E^{(0)}_{0,j}}N_{0,j}J_1(\rho) + \sum_{n=1}^{\infty}C_n\mathcal{J}_{n,j}(\rho) + \sum_{p,n=1}^{\infty}\left(C_{n+p}+C_{|n-p|}\right)\mathcal{J}_{n,j}(\rho)\cos(p\alpha) + \sum_{p=1}^{\infty}\Big\{b_pJ_p(\rho) - \rho a_0C_pJ_1(\rho)\Big\}\cos(p\alpha) \quad (13)$$

where $\mathcal{J}_{n,j}(\rho) = \frac{\rho}{2}\Big\{a_nJ_n'(\rho) - \frac{\rho}{2}N_{0,j}C_nJ_1'(\rho)\Big\}$.
Boundary condition $\psi^{(2)}_{0,j}(R_0,\alpha) = 0$ extracts $E^{(2)}_{0,j}$ as given in (Eq. (12)) and the coefficients $b_p$.

*Case II: Degenerate states* ($l \neq 0$)
In this case, the first order wavefunction correction is given by

$$\psi^{(1)}_{l,j} = \left\{a_lJ_l(\rho) + \frac{\rho N_{l,j}J_l'(\rho)}{2}\left(C_{2l} + \frac{E^{(1)}_{l,j}}{E^{(0)}_{l,j}}\right)\right\}\cos(l\alpha) + \sum_{\substack{p=1\\p\neq l}}^{\infty}\Big\{a_pJ_p(\rho) + \frac{\rho}{2}N_{l,j}J_l'(\rho)\left(C_{l+p}+C_{|l-p|}\right)\Big\}\cos(p\alpha) + a_0J_0(\rho) + \frac{\rho N_{l,j}C_l}{2}J_l'(\rho) \quad (14)$$

Here we have considered only the 'cosine' form of $\psi^{(0)}_{l,j}$ (see Eq. (10)) for the $l\neq 0$ case. The other solution with the $\sin(l\alpha)$ term can be treated similarly. We estimate the first order energy corrections by imposing the boundary condition on $\psi^{(1)}_{l,j}$. $E^{(1)}_{l,j}$ is also verified by substituting $\psi^{(0)}_{l,j}$ in Eq. (9). We have

$$E^{(1)}_{l,j} = -E^{(0)}_{l,j}C_{2l} \quad (15)$$

which is generally non-vanishing unlike the earlier case. The second order energy correction becomes crucial when $C_{2l} = 0$. However, in this work we have not considered this. The choice of the 'sine' solution for $\psi^{(0)}_{l,j}$ (Eq. 10) gives $E^{(1)}_{l,j} = E^{(0)}_{l,j}C_{2l}$.

The coefficients $a_0$ and $a_p$ are obtained by using the boundary condition on $\psi^{(1)}_{l,j}$. This gives us

$$a_0 = -\frac{N_{l,j}\rho_{_{l,j}}C_l}{2}\frac{J_l'(\rho_{_{l,j}})}{J_0(\rho_{_{l,j}})},$$
$$a_p = -\frac{N_{l,j}\rho_{_{l,j}}J_l'(\rho_{_{l,j}})}{2J_p(\rho_{_{l,j}})}\left[C_{p+l}+C_{|p-l|}\right], \quad (p\neq 0,l).$$

The coefficient $a_l$ can be obtained from the normalisation of $\psi^{(1)}_{l,j}$. These results are consistent with the earlier investigations [5].

*Results and Discussions.*— We next apply the formalism developed in the earlier section to a few specific

| **Energy labels** | **Square** | | | **Ellipse** | | | **Supercircle** | | |
|---|---|---|---|---|---|---|---|---|---|
| | $r = \frac{a}{(\lvert\cos\theta\rvert + \lvert\sin\theta\rvert)}$ | | | $r = \frac{a}{\sqrt{1-\varepsilon^2\cos^2\theta}}$ | | | $r = \frac{a}{(\lvert\cos\theta\rvert^t + \lvert\sin\theta\rvert^t)^{1/t}}$ | | |
| | $a = 1$ | | | $a = \sqrt{3}/2 \quad \varepsilon = 0.5$ | | | $a = 1 \quad t = 3$ | | |
| | $R_0 = 0.7935$ | | | $R_0 = 0.9294$ | | | $R_0 = 1.0596$ | | |
| $l, k$ | Es | Ps | % Error | Ns | Ps | % Error | Ns | Ps | % Error |
| 0, 1 | 9.870 | 10.129 | 2.61 | 6.744 | 6.744 | 0.00 | 5.219 | 5.217 | 0.04 |
| 0, 2 | 49.348 | 49.533 | 0.37 | 37.191 | 37.777 | 1.58 | 27.157 | 27.138 | 0.07 |
| 2, 1 | 39.478 | 36.047 | 8.69 | 29.080 | 30.416 | 4.59 | 22.372 | 22.141 | 1.03 |
| 2, 1 | 49.348 | 47.726 | 3.29 | 30.725 | 30.652 | 0.23 | 25.087 | 24.838 | 0.99 |
| 4, 1 | 88.826 | 87.429 | 1.57 | 65.637 | 66.664 | 1.56 | 51.782 | 51.365 | 0.81 |
| 4, 1 | 98.696 | 95.471 | 3.27 | 65.343 | 66.662 | 2.02 | 50.967 | 51.203 | 0.46 |

Table I: Comparison of the first few energy eigenvalues (with the magnitude of % error) for different boundary geometries

boundary geometries. The analysis is restricted to convex domains only to ensure numerical convergence. We have considered the case of a square, an ellipse and a supercircle. The specific form of $r(\theta)$ for these closed curves are used to calculate the metric deformation and thereby estimate energy corrections. The perturbative prescription is seen to converge with dominant non-zero corrections coming from the first few orders. It can be seen that the first and second order corrections in energy are linear and bi-linear in $C_n$ respectively. Further, it is clear that $E^{(m)}$ will be $m$-linear in $C_n$, hence the convergence of the Fourier coefficients, $C_n$, will ensure the convergence of the series. In this analytic formalism the approximation appears only through truncation of the series given by Eqs. (7).

We have estimated energy corrections up to the second order in perturbation for the $l = 0$ states and only first order corrections for the $l \neq 0$ states. The two-fold degeneracy of the original $l \neq 0$ states split at the first order for $C_{2l} \neq 0$. Our results for first few energy levels are summarised in the Table I. The results obtained using the perturbative scheme (Ps) are compared with the numerical (Ns) or exact (Es) solutions. Numerical solutions are obtained using the PDE Toolbox™ of MATLAB®. Our results are in good agreement with the numerical results. The discrepancy is $\sim 5\%$ for the case of the square and $< 1\%$ for the supercircle. The method is expected to yield better results for smooth boundaries without vertices. The results for the supercircle even at the first order show better accuracy than its second order counterpart for the square. However, our method can achieve any desired accuracy by incorporating higher order corrections.

In conclusion we note that Fourier decomposition of the boundary asymmetry makes the method completely general and holds good for a wide variety of boundaries. Since our solutions are general in principle other boundary conditions such as, Neumann, could also be applied to obtain the corresponding spectrum. This makes it crucially important in estimating energy eigenvalues and eigenfunctions for problems.

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